What is claimed is:

Claims

1. A method for use in deriving a chemical structure diagram,

comprising:

5   identifying, from a connection table for a chemical structure, an instance

of chemical structural symmetry in the chemical structure; and

          expressing the instance of chemical structural symmetry in the chemical

structure diagram.

10   2. A method for use in deriving a chemical structure diagram,

comprising:

          determining, from a first chemical structure diagram, a force term for

increasing diagrammatic symmetry within the first chemical structure diagram;

and

15   applying the force term in a derivation of a second chemical structure

diagram from the first chemical structure diagram, the second chemical structure

diagram having more diagrammatic symmetry than the first chemical structure

diagram.

3. A method for use in deriving a chemical structure diagram,
comprising:

determining, from a first chemical structure diagram, a parameter for use
in producing the shape of an addition to the first chemical structure diagram;

5 producing the shape of the addition based on the parameter; and

producing a second chemical structure diagram by adding the addition to
the first chemical structure diagram.

4. A method for use in deriving a chemical structure diagram,
10 comprising:

determining a first rectangle that defines a first portion of an available
layout area, the first rectangle being of a sufficient size to enclose a first chemical
structure diagram;

determining a second rectangle that defines a second portion of an
15 available layout area, the second portion being non-overlapping with the first
portion, the second rectangle being of a sufficient size to enclose a second
chemical structure diagram; and

positioning the first and second chemical structure diagrams within the
first and second portions, respectively.

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5. A system for use in deriving a chemical structure diagram, comprising:

an identifier identifying, from a connection table for a chemical structure,

an instance of chemical structural symmetry in the chemical structure; and

an expressor expressing the instance of chemical structural symmetry in

5   the chemical structure diagram.

6. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a force

term for increasing diagrammatic symmetry within the first chemical structure

10   diagram; and

an applicator applying the force term in a derivation of a second chemical

structure diagram from the first chemical structure diagram, the second chemical

structure diagram having more diagrammatic symmetry than the first chemical

structure diagram.

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7. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining, from a first chemical structure diagram, a

parameter for use in producing the shape of an addition to the first chemical

structure diagram; and

a producer producing the shape of the addition based on the parameter

and producing a second chemical structure diagram by adding the addition to

the first chemical structure diagram.

5   8. A system for use in deriving a chemical structure diagram, comprising:

a determiner determining a first rectangle that defines a first portion of an

available layout area, the first rectangle being of a sufficient size to enclose a

first chemical structure diagram, the determiner determining a second rectangle

that defines a second portion of an available layout area, the second portion

10   being non-overlapping with the first portion, the second rectangle being of a

sufficient size to enclose a second chemical structure diagram; and

a positioner positioning the first and second chemical structure diagrams

within the first and second portions, respectively.

15   9. Computer software, residing on a computer-readable storage medium,

comprising a set of instructions for use in a computer system to help cause the

computer system to derive a chemical structure diagram, the instructions

causing the system to:

identify, from a connection table for a chemical structure, an instance of

20   chemical structural symmetry in the chemical structure; and

express the instance of chemical structural symmetry in the chemical

structure diagram.

10. Computer software, residing on a computer-readable storage

5   medium, comprising a set of instructions for use in a computer system to help

cause the computer system to derive a chemical structure diagram, the

instructions causing the system to:

determine, from a first chemical structure diagram, a force term for

increasing diagrammatic symmetry within the first chemical structure diagram;

10   and

apply the force term in a derivation of a second chemical structure

diagram from the first chemical structure diagram, the second chemical structure

diagram having more diagrammatic symmetry than the first chemical structure

diagram.

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11. Computer software, residing on a computer-readable storage

medium, comprising a set of instructions for use in a computer system to help

cause the computer system to derive a chemical structure diagram, the

instructions causing the system to:

determine, from a first chemical structure diagram, a parameter for use in

producing the shape of an addition to the first chemical structure diagram;

produce the shape of the addition based on the parameter; and

produce a second chemical structure diagram by adding the addition to

5   the first chemical structure diagram.

12. Computer software, residing on a computer-readable storage

medium, comprising a set of instructions for use in a computer system to help

cause the computer system to derive a chemical structure diagram, the

10   instructions causing the system to:

determine a first rectangle that defines a first portion of an available

layout area, the first rectangle being of a sufficient size to enclose a first chemical

structure diagram;

determine a second rectangle that defines a second portion of an available

15   layout area, the second portion being non-overlapping with the first portion, the

second rectangle being of a sufficient size to enclose a second chemical structure

diagram; and

position the first and second chemical structure diagrams within the first

and second portions, respectively.

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